

FIG. 1

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graph TD
    20[COMPARE ALL MOLECULES  
IN A TRAINING SET OF N MOLECULES  
TO EACH OTHER ACCORDING TO  
A STRUCTURAL SIMILARITY METRIC] --> 22[SELECT A DTC MOLECULE  
FROM THE TRAINING SET]
    22 --> 24[SORT ALL OTHER MOLECULES IN  
THE TRAINING SET IN DESCENDING  
ORDER OF STRUCTURAL SIMILARITY  
TO THE SELECTED DTC MOLECULE]
    24 --> 26[COMPUTE A FRACTION CORRECTLY  
PREDICTED METRIC FOR EACH OF  
THE SORTED TRAINING MOLECULES]
    26 --> 27[SELECT ONE OR MORE FRACTION CORRECTLY  
PREDICTED THRESHOLDS]
    27 --> 28[COUNT THE NUMBER OF MOLECULES  
AWAY FROM THE DTC MOLECULE AT WHICH  
THE ACTUAL FRACTION CORRECTLY  
PREDICTED DROPS BELOW THE THRESHOLDS]
    28 --> 30{LAST DTC MOLECULE  
?}
    30 -- NO --> 22
    30 -- YES --> 34[CHOOSE AS MARKER MOLECULES  
THOSE DTC MOLECULES FOR WHICH  
THE FRACTION CORRECTLY PREDICTED  
EXCEEDS A THRESHOLD FOR A  
SELECTED MINIMUM NUMBER OF MOLECULES]
  
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FIG. 2

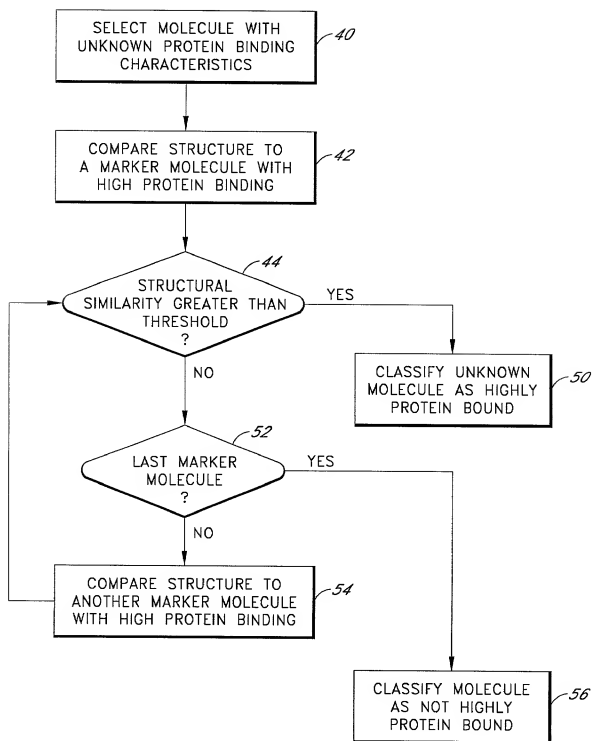


FIG. 3

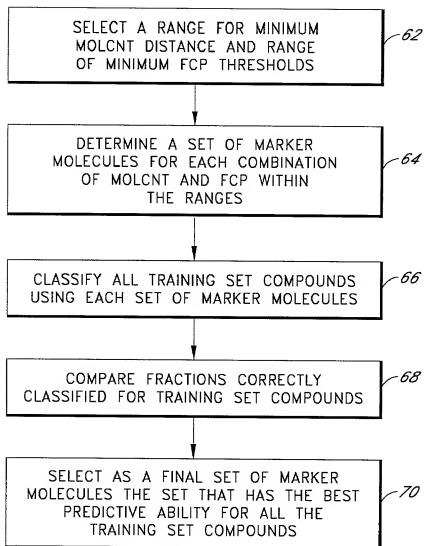


FIG. 4

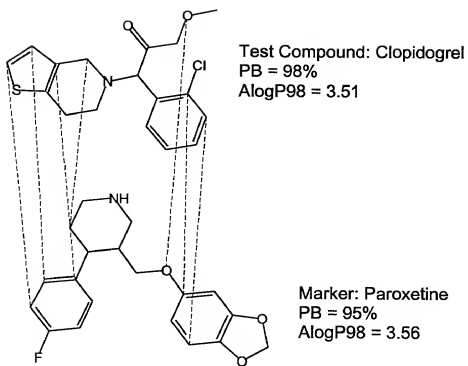


FIG. 5